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Abstract

Boundary-value problems involve two dependent variables: a potential function, and a stream function. They can be approached in two mutually independent ways. The first, introduced by Laplace, involves spatial gradients at a point. Inspired by Faraday, Maxwell introduced the other, visualizing the flow domain as a collection of flow tubes and isopotential surfaces. Boundary-value problems intrinsically entail coupled treatment (or, equivalently, optimization) of potential and stream functions. Historically, potential theory avoided the cumbersome optimization task through ingenious techniques such as conformal mapping and Green's functions. Laplace's point-based approach, and Maxwell's global approach, each provides its own unique insights into boundary-value problems. Commonly, Laplace's equation is solved either algebraically, or with approximate numerical methods. Maxwell's geometry-based approach opens up novel possibilities of direct optimization, providing an independent logical basis for numerical models, rather than treating them as approximate solvers of the differential equation. Whereas points, gradients, and Darcy's law are central to posing problems on the basis of Laplace's approach, flow tubes, potential differences, and the mathematical form of Ohm's law are central to posing them in natural coordinates oriented along flow paths. Besides being of philosophical interest, optimization algorithms can provide advantages that complement the power of classical numerical models. In the spirit of Maxwell, who eloquently spoke for a balance between abstract mathematical symbolism and observable attributes of concrete objects, this paper is an examination of the central ideas of the two approaches, and a reflection on how Maxwell's integral visualization may be practically put to use in a world of digital computers.

“The formulation is equivalent to the more usual formulations. There are, therefore, no fundamentally new results. However, there is a pleasure in recognizing old things from a new point of view. Also, there are problems for which the new point of view offers a distinct advantage”

Richard Feynman, introducing non-relativistic quantum mechanics, 1948, p. 367

Introduction

Pierre Simon Laplace first used the equation,

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0 \quad , \quad (1)$$

in his study of stability of Saturn’s rings (Laplace, 1787). Here V is a scalar function, twice differentiable in space. Soon, the equation was extended to electrostatics by Poisson, and heat by Fourier. During the 1850s, Riemann made major advances in the application of complex variable theory to two-dimensional boundary-value problems. Contemporaneously, Maxwell, inspired by Faraday’s intuition, introduced a radically new way of appreciating boundary-value problems by looking at flow systems as a whole, rather than continuity at a point, by introducing concepts of flow lines and flow tubes. During the second half of the 19th century, complex variable theory inspired important applications in electromagnetism and fluid mechanics, notably in the form of conformal mapping and flow-net analysis.

Two related developments merit mention. Ohm (1827) expressed galvanic current in terms of spatial difference in potential, and resistance along flow path. In doing so, he departed from Poisson and Fourier who had used gradient at a point to quantify force or flux. Fick (1855) proposed a one-dimensional form of Laplace’s equation, accounting for variation of cross section along flow path.

This paper places the two independent approaches in mutual perspective. The motivation is three-fold. First, for practicing scientists, the insights of the past point to the future. The foundations of many mathematical methods routinely used today were laid during the 19th century, and were invariably presented against a backdrop of intuitive physical underpinnings. A study of these early

contributions is remarkably illuminating. Second, as hydrogeologists, we know from experience that even the sophisticated mathematical model can only provide insights about expected patterns of behavior of earth systems under idealized conditions. Success in using these models depends on our ability to bridge the gap between idealization and observation through judgement stemming from experience. Finally, as participants in the larger scientific venture, we must borrow ideas and methods from other fields as freely as we are in sharing with them the broader significance of our findings in the earth sciences.

Historical Background

Poisson and Fourier

In 1812, Poisson invoked Laplace's procedure to develop a model for electrostatics. His goal was to calculate equilibrium charge distribution on the surface of an electrical conductor so as to simulate Coulomb's experimental observations. Poisson treated force at a point as a partial derivatives of "a certain function", which Green in 1828 referred to as a "potential" (Hofmann, 1996).

A decade later, Joseph Fourier presented the heat equation, with the Laplacian of temperature set equal to its time derivative. This equation reduces to the Laplace equation if the time derivative vanishes. Both Laplace and Poisson dealt with action at a distance between discrete bodies, with the forces of attraction conforming to the inverse square law, according to which force intensity is inversely proportional to distance. Fourier abandoned action-at-a-distance, and introduced the new idea of a continuum, assuming that the change of temperature at a point was dependent only on the point immediately preceding it (Grattan-Guinness, 1972). Later, Maxwell (1864) demonstrated that Fourier's continuum approach also yields the inverse square law. Thus, the Laplacian operator is meaningful both for action at a distance and for a continuum.

Riemann's Two-Variable Model

During the 1850s, Riemann considered two-dimensional boundary-value problems in terms of a potential function and a stream function. The ideas were based on geometric concepts associated with Riemann surfaces. The Cauchy-Riemann Conditions express the coupling between potential function ϕ and stream function ψ ,

$$\frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial y} , \quad and \quad \frac{\partial \phi}{\partial y} = - \frac{\partial \psi}{\partial x} . \quad (2)$$

Riemann also made extensive use of the Dirichlet Principle, which states that a function u which minimizes the integral,

$$\int_V |\nabla u|^2 dV \quad (3)$$

is harmonic, which by definition, is a solution of the Laplace equation.

Together, potential and stream functions constitute a conjugate pair, manifesting as an orthogonal grid of flow lines and iso-potential lines. Geometrically, the theory of analytic functions explores how such an orthogonal grid may behave under distortion and stretching while preserving local angular relationships. Thus, mathematics focuses on the relation between algebraic functions and geometry.

Implicit here is the assumption that the flow domain is occupied by a single material. Consequently, ϕ is a velocity potential, whose gradient at a point constitutes velocity. However, in heterogeneous systems composed of more than one material offering different resistances to flow, a velocity potential has to be replaced by a more general energy potential (Hubbert, 1940). To apply Laplace's equation to heterogeneous media, it is necessary to introduce the parameter conductivity, K , and Laplace's equation takes the widely used form,

$$\nabla \cdot K \nabla \phi = 0 . \quad (4)$$

By definition, K is independent of potential in Laplace's equation which is a linear partial differential equation. When K is a function of potential, (4) becomes non-linear, and is no more considered to be Laplace's equation.

Maxwell's Dynamical Model

In 1855, James Clerk Maxwell ventured to integrate electrostatics, electrodynamics, and electrical induction, using Fourier's heat equation as a metaphor (Maxwell, 1864, Narasimhan, 2003). Inspired by Faraday's intuitive concept of lines of force around a magnet (Figure 1), he visualized electricity as a fictitious incompressible fluid flowing in a resistive medium, driven by spatial variation of pressure. However, Faraday's lines merely represented trajectories of force, and said nothing about their magnitudes. To account for magnitude, Maxwell considered the space between neighboring flow lines, designated as a flow tube. Variation of flow velocity (volumetric flow per unit area per unit time) along a tube of variable cross section was then considered analogous to the variation of the magnitude of force. It is easy to see that if the fluid is injected at a uniform rate at a point in an infinite three-dimensional medium, flow will be spherically symmetric, and velocity will decrease inversely as the square of distance away from the point because surface area of a sphere is $4\pi r^2$.

Figure 1: Lines of force around a magnet, as indicated by alignment of iron filings (From Faraday, 1855, Pl. IV, Fig. 2)

Maxwell imagined the flow domain as being pervaded by a number of flow tubes (Figure 2), each originating at a boundary segment with a prescribed pressure, and ending at another segment with a lower pressure. The volumetric flow rate through each flow tube is constant. No flow occurs between neighboring flow tubes across a flow line. Pressure continuously decreases along the flow tube, in the direction of flow. Surfaces of equal pressure are everywhere perpendicular to flow lines. Along a flow tube, impelling forces arising from pressure decrease are exactly balanced by resistive forces proportional to flow rate, maintaining dynamic equilibrium.

Maxwell defined a unit flow tube as one through which a unit volume of fluid flows in unit time. Within the unit flow tube a unit cell is a segment whose bounding iso-pressure surfaces differ in magnitude by unity. Maxwell reasoned that the work done in moving the fluid through a unit cell is unity. Clearly, the total number of unit cells over the flow domain is equal to the total work done in moving the fluid through the resistive domain. At this point, Maxwell could well have invoked the law of least action and articulated a variational statement of the boundary-value problem, stating that the correct solution to the boundary-value problem is that particular flow configuration for which the total work done is a maximum for the prescribed boundary potentials. Such a statement

would have provided a fully self-consistent, integral description of the boundary-value problem, independent of the differential equation. Remarkably, Maxwell did not do so. Instead, he went on to show that the global representation was reducible to the Laplace equation.

Figure 2: Flow domain pervaded by flow tubes and isopotential surfaces as conceived by Maxwell

Further, Maxwell considered heterogeneous media and anisotropic media. He showed that at an interface between two different materials, flow lines will refract, much like refraction of light paths at interfaces of materials of contrasting refractive indices. The difference was that refraction of flow lines was governed by a tangent law, while refraction of light paths was governed by a sine law (Snell's Law). Also, drawing upon Stokes' work on heat flow in crystals, Maxwell extended Laplace's equation to anisotropic media. In retrospect, Maxwell's physical visualization and Riemann's geometrization of algebraic functions were equivalent, analogous concepts.

Ohm and Fick

Ohm and Fick were experimentalists who brought unique observational insights into understanding steady-state diffusion, although both were admittedly inspired by Fourier's mathematical treatment of heat. Ohm (1827), chose to express electrical current in terms of potential difference over a finite distance, rather than potential gradient at a point. In doing so, he introduced the concept of resistance, governed by the shape and size of the medium and its ability to resist electricity. For prisms of uniform cross section, resistance proved to be,

$$R = \frac{\sigma L}{A} , \quad (5)$$

where R is resistance, L is the length of the prism, A is cross sectional area, and σ is the resistivity of the material. Ohm viewed the prism as a flow tube, as was done later by Maxwell.

Fick (1855) conducted molecular diffusion experiments in a container of truncated conical shape, with cross section varying along flow path. To interpret the observations, he expressed the Laplace equation in one dimension thus,

$$K \left(\frac{d^2 \phi}{dx^2} + \frac{1}{A} \frac{dA}{dx} \frac{d\phi}{dx} \right) = 0 \quad , \quad (6)$$

where K is the diffusion coefficient, and A is the spatially variable area of cross section. Fick's equation is applicable in general to an arbitrary flow tube, described with a curvilinear x-axis (Figure 3), and bounded at inlet and outlet by surfaces of equal concentration.

Figure 3: Flow tube of variable cross section. One of the flow paths constitutes a curvilinear x-axis. A(x) denotes area of the isopotential surface passing through x

The exact solution of this equation is,

$$\phi(x) = \phi_{inlet} - m(\phi_{inlet} - \phi_{outlet}) \quad , \quad (7)$$

where, m is the ratio of the resistance of the flow tube between inlet and x, and the total resistance from the inlet to outlet. The resistance of the flow tube between two positions x_1 and x_2 is given by,

$$R_{x_1, x_2} = \int_{x_1}^{x_2} \frac{dx}{K A(x)} \quad . \quad (8)$$

The presence of K in the integrand indicates that (8) is quite general in its scope and is applicable to heterogeneous media, as well as for non-linear problems. In heterogeneous media, flow lines will refract at material interfaces, causing the flow tube to bend.

Second Half of 19th Century

During the second half of the nineteenth century, Riemann's work led to important developments in the solution of steady-state flow problems in two dimensions. Notable among these were conformal mapping and flow-net analysis. Conformal mapping consists in mapping a given flow domain into one of simpler flow symmetry that is amenable to easy mathematical treatment. The

solution so obtained is then inverted back to the real domain.

Two-dimensional boundary-value problems with flow domains of complex shape can be graphically solved in some cases with flow-nets. The approach is to fill the flow domain, by trial and error, with an orthogonal network of flow lines and isopotential lines, drawn on paper according to specified rules. In practice, the flow domain is divided into a set of curvilinear squares, using a soft pencil and an eraser. When finished, the flow net consists of a collection of flow tubes, each divided into equal intervals of potentials between inlet and outlet.

Solving Boundary-Value Problems

Mathematically, solving Laplace's equation implies the task of finding a continuous function ϕ which satisfies the Laplace equation in the interior, and the prescribed conditions on the boundary. The geometric configuration of the closed boundary, and the prescribed boundary conditions are described with algebraic functions, regardless of numerical magnitudes. Solutions obtained for these problems may be exact functions, infinite sums or other approximations. Experience shows that solving boundary-value problems algebraically is realizable only for certain classes of problems with relatively simple geometric configurations and associated boundary conditions. Problems involving more complex geometrical shapes, heterogeneity, and mixed boundary conditions that are not amenable to solution by algebraic methods are posed as case-specific numerical problems, to be solved using numerical methods. The advantage of algebraic methods is that they provide generic insights about classes of problems, without having to describe individual problems numerically. The limitation is that complex problems typical of real-world situations cannot often be so solved. Numerical methods, though helpful in solving realistic, complex problems, cannot provide general insights as effectively as analytical solutions. The two approaches, therefore, constitute complementary tools.

It is useful to examine boundary-value problems systematically, from the simplest case of purely unidirectional flows, through perturbed unidirectional flows, to asymmetrical flows in symmetrical objects, and finally to general non-symmetric flows involving multiple inlets and outlets.

Purely Symmetrical Flows

The simplest flow domains are those in which the flow trajectory parallels one of the coordinate

axes, as for example, flow through a rod or prism of finite length, radial flow through a cylindrical annulus, or flow through a spherical shell (Figure 4, A, B). In these cases, the entire domain may be considered to be a single large flow tube.

Figure 4: Examples of symmetric flows: (A) Rod or prism of uniform cross section, and (B) Flow away from the axis of a cylinder, or flow away from center of sphere

For these cases, $A(x)$ is equal, respectively, to a constant, $2\pi x$, and $4\pi x^2$. For each of these cases, the flux J_x through the tube is given by, $(\phi_{in} - \phi_{out})/R$, where R is given by (8).

A more complicated symmetrical flow pattern involves elliptic cylindrical coordinates (Figure 5). Consider a flow system in which potentials are prescribed on an inner ellipse and an outer ellipse of a set of confocal ellipses. The flow trajectories in such a system are along hyperbolas that are normal to the ellipses representing surfaces of equal potential. The set of confocal ellipses are defined by the distance $2d$ between their foci. The coordinates ξ and η of the elliptical coordinate system are related to the Cartesian coordinates r and x by,

$$x = d \sqrt{(\xi^2 - 1)(1 - \eta^2)} \quad \text{and} \quad z = d \eta \xi, \quad (9)$$

where $\eta = \cos \theta$, and θ is the angle between the z -axis and the asymptote to the hyperbola. The ranges of the coordinates are $1 \leq \xi < \infty$, and $-1 \leq \eta \leq 1$.

Figure 5: Flow in a system with elliptical symmetry. Flow lines are hyperbolas normal to the confocal ellipses

Assume for convenience that the potential on the inner ellipse is higher than that on the outer ellipse, with flow directed away from the center, and the hyperbolas forming flow lines. The confocal ellipses between inlet and outlet constitute isopotential surfaces. Let one of these hyperbolas be chosen as a curvilinear x -axis. Then, using the relations given in (9), one can generate an expression $A(x)$ for the surface areas of the elliptical cylinders as a function of distance along the chosen curvilinear x -axis. This $A(x)$, in conjunction with (7) then helps evaluate ϕ as a function of x . Alternatively, the problem can also be solved in elliptic cylindrical coordinates, to yield solutions

involving Mathieu functions (Wolfram Math World, 2006).

Total flux calculation for this system is more involved than in the previous cases. Note that the length of flow trajectories between any two confocal ellipses varies as a function of the asymptotic angle θ of the hyperbolas. The question arises as to which of the trajectories one should use as the curvilinear x-axis to get the correct total flux. Now, since the collection of flow tubes constitutes a parallel flow system, the trajectory chosen must be such that its length between the inlet and the outlet is the arithmetic mean of the lengths of all the trajectories.

Perturbed Unidirectional Flows

Figure 6A shows a unidirectional flow system in which a linear flow pattern is diverted around a cylindrical obstruction. With the help of conformal mapping, this flow pattern can be transformed into a simple linear flow pattern as indicated in Figure 6B. Conformal mapping transforms the curvilinear orthogonal grid in the vicinity of the cylinder into a rectilinear grid. The known analytical solution for the rectilinear grid can be transformed back to the real domain through appropriate inverse transformation.

Figure 6: Example of conformal mapping: A. Unidirectional flow deflected around a cylinder, B. Linear flow in the transformed domain

Flow of water through the foundation below a concrete dam is shown schematically in Figure 7A. Water enters the foundation from the reservoir on the upstream side of the dam, and it leaves the foundation on the downstream side. In between, the flow pattern is perturbed by a cut-off wall. The flow is unidirectional. This boundary-value problem can be graphically solved by drawing a flow-net, as shown in Figure 7B.

Figure 7: Seepage of water under a concrete dam with cut-off wall (A) Schematic description, (B) Flow net

Superposition of Elementary Solutions

A powerful approach to solve Laplace's equation is the superposition of elementary solutions of systems with simple flow symmetry, using Fourier series or Green's functions. Superposition is

possible because Laplace's equation is a linear partial differential equation. This approach is advantageous when the flow domain has a regular shape such as cylinder or a sphere, and non-symmetrical flows result from non-uniform boundary conditions.

Fourier Series

Consider a circular flow domain (Figure 8) of radius r_e with an inner circular boundary of radius r_w . The potential is constant along the inner circle, and is prescribed on the outer boundary to be, $f(\theta) = 0$, $-\pi < \theta < 0$, and $f(\theta) = \theta$, $0 \leq \theta \leq \pi$.

Figure 8: Concentric flow domain with asymmetrical boundary conditions. Angle θ is measured counter clockwise from B. At A, $\theta = \pi$

In radial coordinates, Laplace's equation for this problem is given by,

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} = 0 \quad . \quad (10)$$

This problem involves non-symmetrical flow patterns with ϕ dependent both on r and on θ . Equation (10) has several elementary solutions (Muskat, 1937),

a constant, $\ln r$, $r^\alpha \cos \alpha\theta$, $r^\alpha \sin \alpha\theta$, $r^{-\alpha} \cos \alpha\theta$, and $r^{-\alpha} \sin \alpha\theta$

The general solution for (10) can be written as a superposition of all these solutions,

$$\phi = c_0 \ln r + \sum r^\alpha (a_\alpha \sin \alpha\theta + b_\alpha \cos \alpha\theta) + \sum r^{-\alpha} (c_\alpha \sin \alpha\theta + d_\alpha \cos \alpha\theta) \quad . \quad (11)$$

In (11) the coefficients, c_0 , α , a_α , b_α , c_α , and d_α are all constants. To determine these constants, the known conditions on the inner boundary and the outer boundary are expressed as infinite Fourier series involving sines and cosines. Solving the resultant equations yields all the relevant

coefficients.

Poisson's Formula

Poisson's formula provides a way of finding the potential at a point within closed flow domains in the interior of which Laplace's equation is satisfied, and potentials are prescribed all along the closed boundary. One starts with the premise that the potential at a point of interest P is a weighted integral of the prescribed boundary potentials. Thus,

$$\phi(P) = -\frac{1}{2\pi} \int_{\sigma} \phi(Q) w(Q) d\sigma, \quad (12)$$

where $w(Q)d\sigma$ is the weight associated with the potential at point Q on the boundary. In Poisson's formula, the weighting function is chosen to be the normal derivative at Q of the Green's Function for the pair of points P and Q.

Accordingly, Poisson's formula is written as,

$$\phi(P) = -\frac{1}{2\pi} \int_{\sigma} \phi(Q) \frac{\partial G(P,Q)}{\partial n} d\sigma. \quad (13)$$

The Green's Function $G(P,Q)$, specific to the pair of points P and Q, involves a unit source located at P in an infinite region, and other unit sources and sinks suitably distributed in such a way that when the effects of these sources and sinks are summed for point Q, the potential at point Q is zero, as long as Q is located anywhere on the boundary. In the Green's function approach, the finite domain of the bounded flow system is replaced by an infinite domain. The cumulative effects of the sources and sinks is to create zero potential at points that occupy positions on the trace of the physical boundary. The product of the normal derivative of the Green's function at a point Q on the boundary and differential area $d\sigma$ gives the magnitude of flux at Q that would occur if the potential were zero everywhere on the boundary, and a unit source were placed at P. To get the potential at P, the potential at Q is weighted by this magnitude.

Domains with Arbitrary Shape and Multiple Boundary Conditions

The most general class of boundary-value problems involve flow domains with arbitrary asymmetrical shape, and mixed boundary conditions, with potentials and/or fluxes specified on three or more boundary segments. Additional complexities may be introduced by heterogeneities. An example (Figures 9A and 9B) is a two-dimensional domain with potentials specified over three segments, with conditions of no-flow prescribed over the rest of the boundary. This is a mixed boundary-value problem. One of the segments has a high potential, the second has an intermediate potential, and the third segment has a low potential. Without actually solving this problem, it is useful to look at its special attributes.

Figure 9: Flow domain with potentials prescribed on three boundary segments may host very different flow patterns (A) two inlets and one outlet, or (B) One inlet and two outlets

At the outset it is clear that the segment with the highest potential must be an inlet, and that with the lowest potential must be an outlet. Whether the segment with the intermediate potential constitutes an inlet or an outlet is not known a priori. It is likely that if the intermediate potential were closer in magnitude to the high potential, the segment will be an inlet (Figure 9A). Or, it will be an outlet if the intermediate potential were closer in magnitude to the low potential (Figure 9B). Obviously, the flow pattern will depend upon the magnitude of the intermediate potential relative to the other two. It follows that a full description of this problem requires prescription of numerical magnitudes of boundary values.

In the format of differential equations, a full description of this two-dimensional problem consists of four elements.

$$\begin{aligned}\nabla^2 \phi &= 0, \\ \nabla^2 \psi &= 0, \\ \text{Cauchy - Riemann conditions, and} \\ \text{Numerical magnitudes of boundary potentials} &.\end{aligned}\tag{14}$$

This is a coupled problem, which cannot be solved algebraically. How then may it be solved? The common approach is to solve for potentials using finite difference, finite volume, or finite element

methods. However, note from (14) that the stream function also satisfies the Laplace equation. Thus, Laplace's equation can also be solved for the stream function, rather than for potentials. As shown by Frind and Matanga (1985), solving for the stream function may be desirable when accurate estimates of velocities are needed for contaminant transport modeling.

The Optimization Problem and its Relation to Variational Principle

We now look at the general boundary-value problem from a global perspective. The approach is to abandon the notions of a point and gradient at a point. Instead, difference in potential over a finite distance, in conjunction with the format of Ohm's Law, forms the basis of analysis.

We postulate that the system, responding to prescribed boundary conditions, organizes itself into the most efficient flow configuration. Here, "efficient configuration" implies either getting a maximum amount of work done for a given set of boundary potentials, or expending a least amount of energy in pushing prescribed fluxes through the flow domain. Achieving such an efficient flow configuration is referred to as least action. This postulate can be expressed mathematically as shown below, with water, the permeant, flowing through a resistive medium.

Following Maxwell (1864), let the flow domain be divided into a conveniently large number of flow tubes, $i = 1, 2, 3, \dots, I$, each with cross sections varying along curvilinear x axes (Figure 3). Then, in the format of Ohm's Law, the mass of water flowing through tube i in unit time is,

$$J_i = \frac{(\phi_{in} - \phi_{out})_i}{R_i}, \quad (15)$$

where J_i is the mass of water flowing through the i^{th} flow tube in unit time, R_i is the hydraulic resistance offered by the tube as defined in (8), and ϕ is the hydraulic potential, defined to be energy per unit mass of water. It follows that the mass of water entering the flow tube brings in energy, and the mass of water flowing out carries energy out of the system. The net energy excess of inflow over outflow is consumed in doing work against frictional resistance. Thus, W_i , the work done per unit time in moving water through flow tube, is,

$$W_i = J_i (\phi_{in} - \phi_{out})_i = \frac{(\phi_{in} - \phi_{out})_i^2}{(R_i)_{in,out}} . \quad (16)$$

Then, the total energy expended per unit time over the entire domain is,

$$W_{Total} = \sum_{i=1}^I \frac{(\phi_{in} - \phi_{out})_i^2}{(R_i)_{in,out}} . \quad (17)$$

The flow configuration for which W_{Total} is a maximum for a prescribed set of boundary potentials constitutes the desired solution.

An alternate way of evaluating W_{Total} is to rewrite (16) as,

$$W_i = J_i (\phi_{in} - \phi_{out})_i = J_i^2 (R_i)_{in,out} \quad (18)$$

Note that (18) has the same form as Joule's law, stating that heat generated by an electrical resistor equals the square of the current times resistance. The total work done is then given by,

$$W_{Total} = \sum_{i=1}^I J_i^2 (R_i)_{in,out} . \quad (19)$$

If one chooses to use (18) to evaluate the work done, then the flow configuration for which (19) is a minimum constitutes the desired solution. The physical significance of (17) and (19) is as follows. For a prescribed set of potentials on the boundary, the system adjusts itself to maximize work done.

Or, for a prescribed set of fluxes, the system adjust itself to maintain the fluxes with a minimum amount of work. For the simple case of a system with one inlet and one outlet, both (17) and (19) are equivalent to finding the flow configuration with least total resistance.

It is pertinent to examine how the optimization problem relates to a variational statement of the boundary-value problem. Let flow tube i be divided into j segments, each segment being bounded by two surfaces of equal potential. Then, the work done per unit time in moving water through the j^{th} segment is,

$$W_{ij} = \frac{(\Delta \phi_{ij})^2}{R_{ij}} \quad , \quad (20)$$

and, the total work done in flow tube i is,

$$W_i = \sum_{j=1}^J \frac{(\Delta \phi_{ij})^2}{R_{ij}} \quad . \quad (21)$$

Noting that R_{ij} can be expressed as, $\Delta x/(KA)$, that $\Delta V = A \, dx$, and letting $I \rightarrow \infty$ and $J \rightarrow \infty$ we get,

$$\Omega = W_{Total} = \sum_{i=1}^{I \rightarrow \infty} \sum_{j=1}^{J \rightarrow \infty} K \left[\left(\frac{\Delta \phi}{\Delta x} \right)_{ij} \right]^2 \Delta V_{ij} = \int_V K (\nabla \phi)^2 dV \quad . \quad (22)$$

The integral on the right-hand side of (22) represents the variational principle for a heterogeneous medium in which K is spatially variable. If the medium is homogeneous, K is spatially constant, and the domain two-dimensional, (22) reduces to the Dirichlet principle (3). One can readily show by perturbing ϕ and minimizing Ω that one gets the Laplace's equation, $\nabla \cdot K \nabla \phi = 0$. Harmonic functions exist in two and three dimensions. Therefore, Dirichlet principle is valid in general three

dimensions. However, the Cauchy-Riemann conditions are restricted to two dimensions, and methods such as conformal mapping, or solving for the stream function that rely on the Cauchy-Riemann conditions cannot be extended to three dimensions.

What We Know, and What We May Look Ahead To

Laplace's equation states that the divergence of the potential function is equal to zero within a closed domain. Harmonic functions satisfy Laplace's equation. In two dimensions, harmonic functions exist in conjugate pairs. The potential function and the stream function constitute a conjugate pair, and are coupled together by the Cauchy-Riemann conditions. An enormous body of literature exists on potential theory and harmonic functions on theoretical as well as applied aspects of boundary-value problems in two dimensions. A fundamental result of importance on harmonic functions is the Dirichlet Principle (3).

The goal of solving Laplace's equation, is to *find* a harmonic function based on a knowledge of conditions prescribed on the boundary. To this end, one starts with a prior knowledge of the nature of spatial variation of gradients of the desired function over the domain, and integrates them subject to known boundary conditions. In systems with well-defined symmetrical flow patterns, the known flow symmetry provides all the needed information about spatial gradients necessary for integration, leading to an explicit, algebraic solution of Laplace's equation.

However, when the problem is devoid of flow symmetry, adequate information may not be available beforehand on the nature of variation of potential gradients over the flow domain. In such cases, the solution task is beset with imprecision. Some problems (e.g. Figure 9), comprising two or more subsystems of flow may not be amenable to algebraic solutions, and have to be described and solved numerically, on a case by case basis. These general classes of problems lie beyond the scope of algebraic methods. In solving these, the coupling between potentials and flow geometry becomes important.

Over the past five decades, the digital computer has motivated the development of a variety of numerical methods that are designed to solve Laplace's equation in two and three dimensions, over flow domains of arbitrary geometric shape, with heterogeneous distribution of materials in the interior. Contrary to what has been argued above, these methods are noteworthy in disregarding the coupling between potential and stream functions, and numerically solving the Laplace equation just

for the magnitudes of potential with notable “success”. How may we reconcile this apparent contradiction?

These methods (finite difference, finite volume, and finite element) have the goal of calculating the magnitude of potential at a finite number of points within the flow domain of interest, consistent with the prescribed set of boundary conditions. This goal is achieved by assuming that the gradient of potential between neighboring points corresponds to an *a priori* chosen functional form (usually, linear variation of potential with distance). This is clearly an approximation. For, in a flow system involving converging and diverging flow patterns, the gradient at any point is governed by the local flow pattern. Therefore, in the absence of prior knowledge of flow patterns, the boundary-value problem inherently involves two unknowns, namely, the potential function and the stream function. Consequently, “solving” the problem entails optimization, rather than explicitly solving for a single variable. Be this as it may, what is practically relevant in applied problems is acceptable magnitudes of approximation errors. In this sense of acceptable magnitudes of error, the aforesaid methods are successful, as discussed below.

Gradient, by definition, is an infinitesimal concept. If a mathematical function is known *a priori*, its gradient can be evaluated precisely by differentiation. This is a “forward problem”. On the other hand, if the function has to be determined based on its value at discrete points, such a determination will be non-unique and approximate because the gradient in the vicinity of discrete points cannot be uniquely determined. The task of finding the function from a knowledge of its gradients is an “inverse” problem. Only in the limiting case of an infinite number of points filling the entire flow domain, the numerical solution of the inverse problem indicated above will yield the exact solution. In other words, the two-variable problem is reduced to a single-variable problem, without loss of accuracy. In practice, one can fill the domain with a conveniently large number of discrete points (rather than infinite number of points), and still obtain results of acceptable accuracy. In groundwater hydrology, these numerical errors are far smaller than those arising due to a lack of field data. With spectacular developments in computational speed and information storage, numerical models now can handle millions of grid points in a flow domain of interest. From a practical perspective therefore, currently available numerical models are adequate to solve boundary-value problems in two and three dimensions under the most general conditions with acceptable accuracy, solving the Laplace equation just for the potential, disregarding coupling with flow geometry.

Given that existing numerical methods, in conjunction with the digital computer, can provide numerical solutions of acceptable accuracy for the most general boundary-value problems, is there any need to explore alternative ways of solving such problems? From a scientific perspective, a need exists. For, it is in the nature of the scientific enterprise to examine alternate ways of looking at ideas and concepts.

Looking at the present state of understanding of Laplace's equation, two limitations stand out. First, the best available mathematical theory for boundary-value problems, the theory of analytic functions, is restricted to two dimensions. There is no three-dimensional equivalent of the Cauchy-Riemann conditions. If so, what constitutes a good methodology for studying three-dimensional boundary-value problems in general? Secondly, conventional wisdom has it that numerical models are approximate solvers of Laplace's partial differential equation. Is there way to move away from this paradigm and directly formulate a numerical models, independent of the differential equation?

Maxwell's model is based entirely on spatial differences in potential along a flow tube, and resistance offered by the flow tube over finite distances. Therefore, this model enables one to disregard the notions of points, gradients, and Darcy's law, and instead choose to use isopotential surfaces, potential differences and the format of Ohm's law. From this perspective, the multi-dimensional boundary-value problem reduces to a collection of one-dimensional problems that are interlinked through a common constraint. This constraint is manifest in the principle of least action, inherent in the energy optimization statement embodied in (17) and (19). Equivalently, the coupling among the flow tubes is represented by the variational principle (22).

Now, an examination of how this model may form the basis for a numerical solution strategy. In two dimensions, the flow field is represented by an orthogonal grid of isopotential lines and flow lines. In three dimensions the flow domain will be filled with a set of flow tubes or conduits whose cross sections are curvilinear quadrilaterals. At the edges, some tubes may have cross sections that are curvilinear triangles. Each flow tube (Figure 10A) originates at a boundary segment of higher potential (inlet), and end at another boundary segment of lower potential (outlet). For each flow tube, a conveniently chosen flow line serves as a curvilinear x-axis, needed to calculate the resistance of the flow tube according to (8). In so calculating resistance, $A(x)$ is the area of cross section of the isopotential surface passing through x (Figure 10A).

Figure 10: Three-dimensional flow, (A) Two adjoining flow tubes, (B) Discretized volume

elements in curvilinear coordinates

Given the foregoing, the general procedure to be followed in solving the coupled problem is to start with a set of flow tubes whose configuration has been guessed at. Each flow tube starts and ends at a boundary segment. Once the configuration is chosen, the resistance for each tube is readily calculated using (8). Then, using prescribed information on inlet and outlet, the work expended in moving water through flow tube i is readily calculated using (16) or (18). The summation of work done over all the flow tubes gives the total work expended. The next task is to modify the flow configuration and repeat the process systematically until the most efficient configuration for which W_{Total} is an extremum is obtained.

Although the energy minimization approach is attractive from a conceptual perspective, it does not indicate how the flow configuration may be progressively adjusted. Therefore, a workable rationale is necessary to progressively modify the configuration of flow tubes to arrive at an optimal configuration. Two approaches present themselves.

In Figure 10A, two neighboring flow tubes, extending from inlet to outlet are shown, each with its own curvilinear coordinate axis. At any point x along this axis, the cross sectional area $A(x)$ coincides with the area of the isopotential surface that contains the point. Now consider point P in Figure 10A, and the associated isopotential surface of flow tube 1, intersecting the curvilinear coordinate axis at x . Then, since $A(x)$ is known, the magnitude of potential of this isopotential surface can be readily calculated using (7). Similarly, one can estimate the magnitude of potential for point P from the isopotential surface associated with flow tube 2. If the two flow tubes are part of the optimal flow configuration of the boundary-value problem, then the magnitudes of potential for P , estimated from each tube must be exactly equal. If the magnitudes differ, then the configuration will require modification. An examination of the mismatch in potentials estimated in this manner at a convenient number of points along the common interface of adjoining flow tubes can then be used to modify the configuration in some systematic way towards achieving the ultimate goal of optimization.

A second approach consists in dividing the flow domain into a convenient number of volume elements that are curvilinear parallelipeds. These are defined by isopotential surfaces with orthogonal surfaces containing flow lines. A portion of such an assemblage is shown in Figure 10B, a longitudinal section along a plane of flow. Volume element (i,j,k) is connected to volume element

(i-1,j,k) on the upstream side and (i+1,j,k) on the downstream side of flow tube i. If the chosen flow configuration corresponds to the optimal configuration of the boundary-value problem, then, there will be no flow transverse to this primary direction. If the configuration is not optimal, there will be some transverse flow. To detect such flow, element (i,j,k) is also connected to (i,j,k-1) and (i,j,k+1) in the z direction, and (i,j-1,k) and (i,j+1,k) in the y direction (perpendicular to the plane of the paper).

The fluxes into and out of element (i,j,k) in the primary direction of flow, are, in view of Ohm's law,

$$Inflow = \frac{(\phi_{i-1,j,k} - \phi_{i,j,k})}{\int_{x_{i-1,j,k}}^{x_{i,j,k}} \frac{dy}{K A(y)}} = C_{up} (\phi_{i-1,j,k} - \phi_{i,j,k}), \quad (23)$$

$$Outflow = \frac{(\phi_{i,j,k} - \phi_{i+1,j,k})}{\int_{x_{i,j,k}}^{x_{i+1,j,k}} \frac{dy}{K A(y)}} = C_{down} (\phi_{i,j,k} - \phi_{i+1,j,k}),$$

where, C_{up} and C_{down} are conductances. We may write similar expressions for flow in the transverse direction between (i,j,k) and (i,j-1,k), (i,j+1,k), (i,j,k-1), and (i,j,k+1). Note that, as indicated in Figure 10B, in considering flow into volume element (i,j,k) one considers a flow tube bounded by the inlet isopotential surface through the point (i-1,j,k), and the outlet isopotential surface through the point (i,j,k). These points merely indicate the location where the respective isopotential surfaces intercept the coordinate axis. Flow occurs between isopotential surfaces. Thus, the points do not have the same connotation as that of a nodal point for which potentials are calculated in conventional numerical methods.

In view of (23), one may assemble a set of linear equations as is done in standard finite difference models, and solve for the unknown potentials over the flow domain. The calculated potentials will be valid for all points on an isopotential surface. Using these values, the next step is to calculate fluxes across all transverse connections over the flow domain. The magnitude of the transverse fluxes will indicate the extent to which the flow configuration departs from the optimum, and will provide a basis for modifying the flow pattern to efficiently progress towards the optimum configuration. At optimum configuration, transverse fluxes will be negligible over the entire flow domain, and all flow will be channeled through along the primary directions of the flow tubes.

This optimization approach amounts to direct solution of the integral equation, and has the advantage that the solution is automatically verified when the optimal configuration is attained. The numerical model has been formulated directly, independent of a differential equation. Accurate results can be obtained with fairly coarse spatial discretization because information on geometry is beneficially utilized in calculating resistances and conductances. An added advantage is that the method of evaluating conductance in (23) by accounting for flow tubes of variable cross section provides a robust way of handling non-linear problems, even with coarse spatial discretization. Finally, flow tubes associated with the optimum flow configuration can be directly used as the basis for solving contaminant transport problems in which a diffusing profile of a contaminant is progressively displaced along the flow tube.

At present, after solving Laplace's equation with adequately large number of grid points, a common practice is to generate stream lines through post-processing of computed potentials, or to generate velocity fields and other images to help visualize the computational results. Remarkably, it is not recognized that the voluminous amount of information latent the visual images so generated can in fact be beneficially fed back into the calculations to take them to the next level of sophistication. Maxwell's global model provides novel opportunities in this regard.

Concluding Remarks

By convention, boundary-value problems are conceptualized in terms of Laplace's partial differential equation. Even the variational principle for boundary-value problems is often used as an artifact to derive the Laplace equation. In the spirit of science, it is prudent to balance this one-sided view with the geometry-based view pioneered by Maxwell.

Throughout his career, Maxwell not only tried to balance mathematics with observational physics, but also eloquently articulated the need for such a balance. In a lecture delivered at Cambridge, Maxwell (1871) stated,

“It is not till we attempt to bring the theoretical part of our training into contact with the practical that we begin to experience the full effect of what Faraday called “mental inertia” – not only the difficulty of recognising , among the concrete objects before us, the abstract relation which we have learned from books, but the distracting pain of wrenching the mind away from the symbols to the objects, and from the objects back to the symbols. This however is the price we have to pay for new ideas.”

By relying solely on Laplace’s differential equation and the abstract mathematical methods of its solution, we miss the balance that Maxwell spoke eloquently about. Faraday’s simple mental-image of lines of force underlies the highly mathematical concept of a ‘field’ in physics (Harman, 1993). In view of this, our comprehension of boundary-value problems can be enriched if, in addition to using Laplace’s mathematical approach, we devote attention to comprehending these problems based on Maxwell’s physical visualization.

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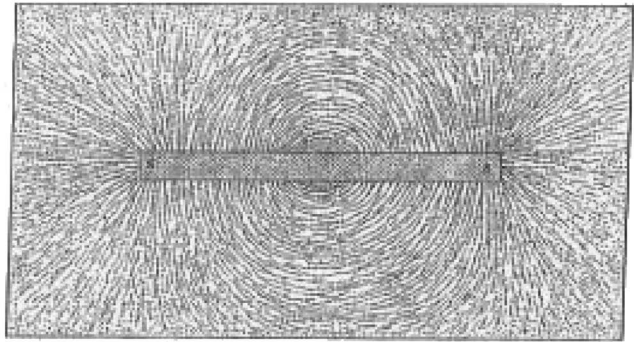
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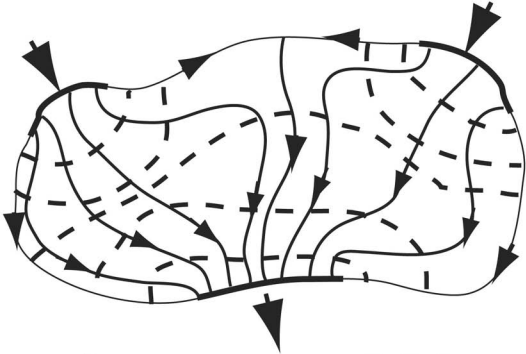
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Figure Captions

- Figure 1: Lines of force around a magnet, as indicated by alignment of iron filings (From Faraday, 1855, Pl. IV, Fig. 2)
- Figure 2: Flow domain pervaded by flow tubes and isopotential surfaces as conceived by Maxwell
- Figure 3: Flow tube of variable cross section. One of the flow paths constitutes a curvilinear x-axis. $A(x)$ denotes area of the isopotential surface passing through x
- Figure 4: Examples of symmetric flows: (A) Rod or prism of uniform cross section, and (B) Flow away from the axis of a cylinder, or flow away from center of sphere
- Figure 5: Flow in a system with elliptical symmetry. Flow lines are hyperbolas normal to the confocal ellipses
- Figure 6: Example of conformal mapping: A. Unidirectional flow deflected around a cylinder, B. Linear flow in the transformed domain
- Figure 7: Seepage of water under a concrete dam with cut-off wall (A) Schematic description, (B) Flow net
- Figure 8: Concentric flow domain with asymmetrical boundary conditions. Angle 2 is measured counter clockwise from B. At A, $2 = B$
- Figure 9: Flow domain with potentials prescribed on three boundary segments may host very different flow patterns (A) two inlets and one outlet, or (B) One inlet and two outlets
- Figure 10: Three-dimensional flow, (A) Two adjoining flow tubes, (B) Discretized volume elements in curvilinear coordinates

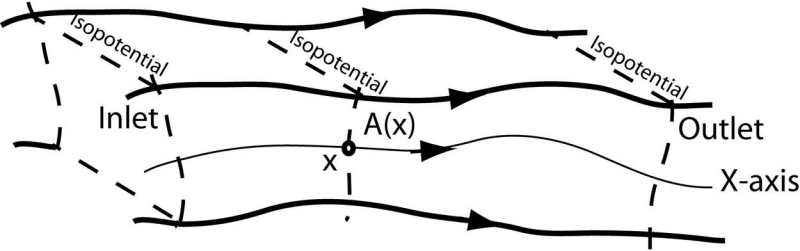


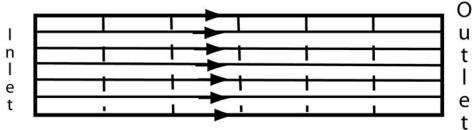



Flow Line

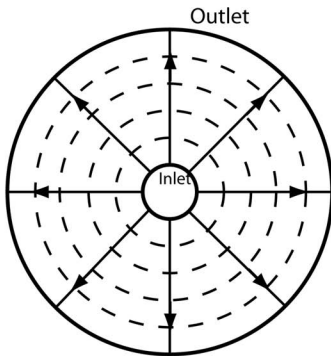
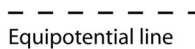
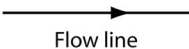

Equipotential Line

 Boundary segment with prescribed potential

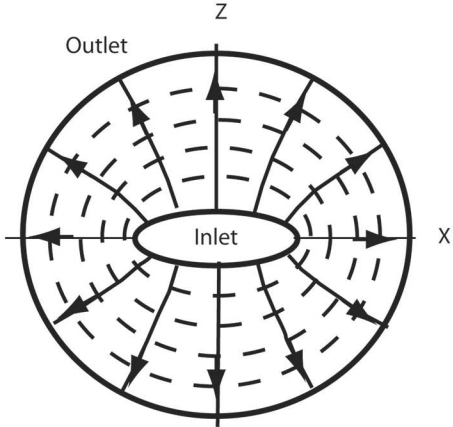




A. Rod or a prism



B. Plan view of a cylinder or Equatorial plane of a sphere



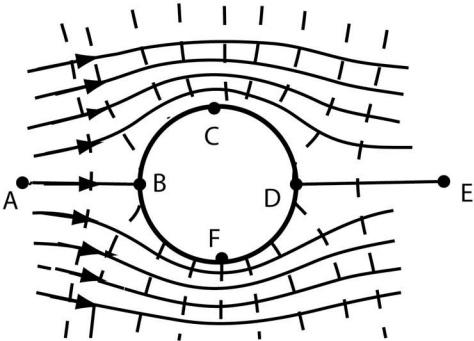
Plan View of an Elliptical Cylinder



Flow lines are hyperbolas



Equipotentials are confocal ellipses



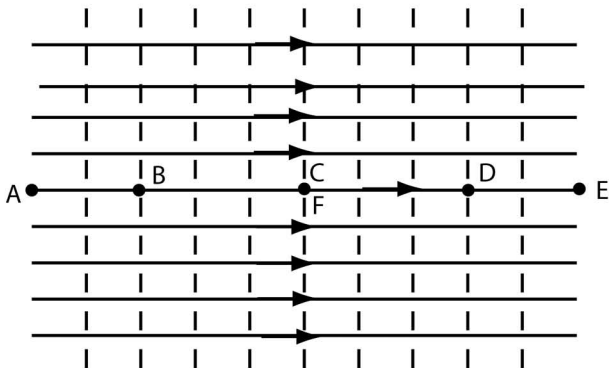
Real Domain



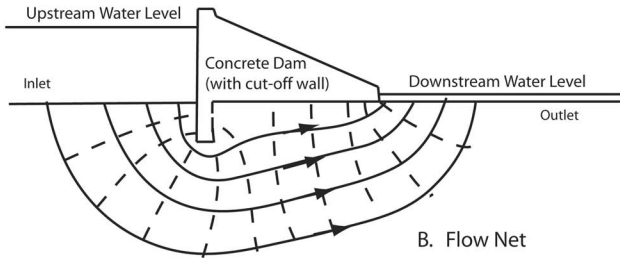
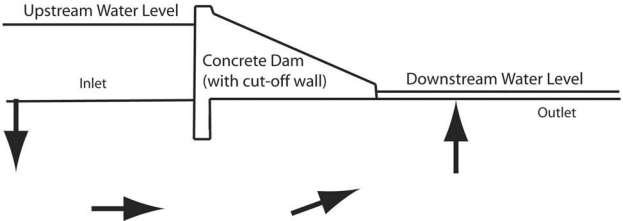
Flow Line

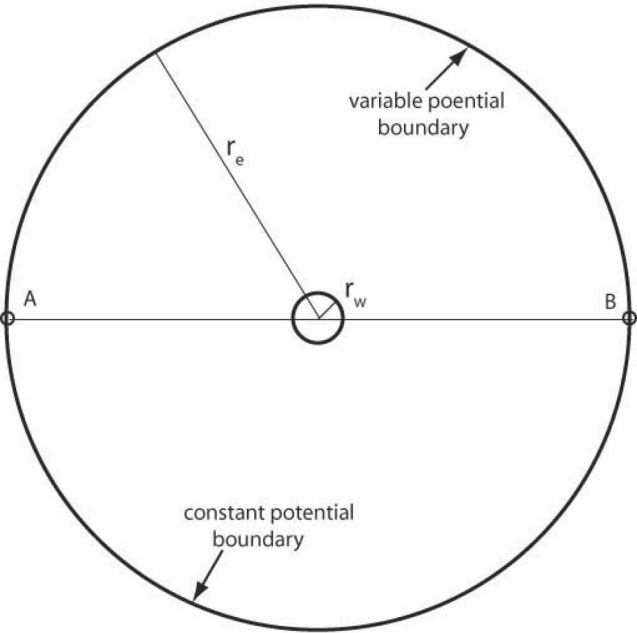


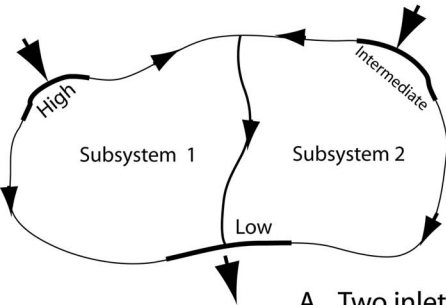
Equipotential Line



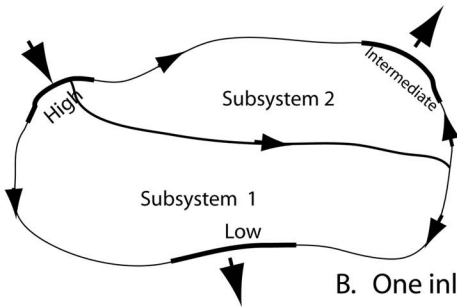
After Conformal Mapping





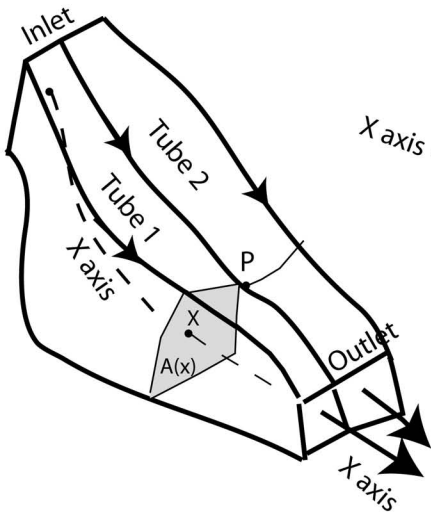


A. Two inlets, One outlet



B. One inlet, Two outlets

A.



B.

